Enhanced Stability and Thermoelectric Figure-of-Merit in Copper Selenide by Lithium doping

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Supporting Information

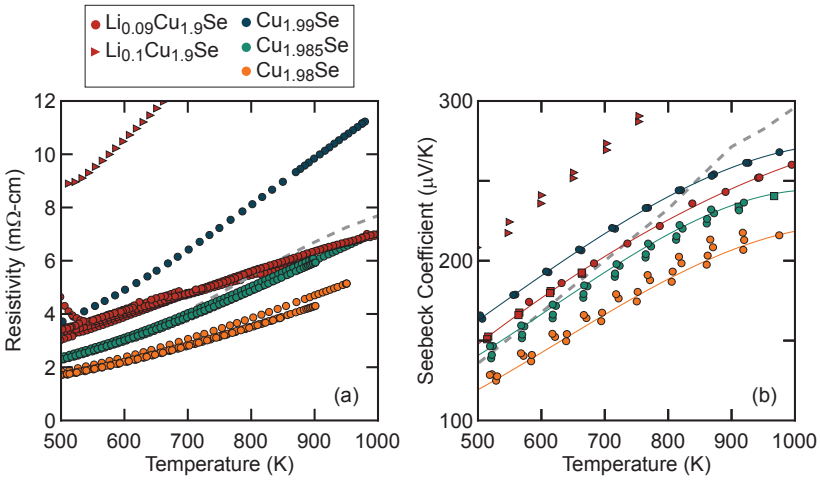

Figure S1: Transport properties of $Cu_{2-x}Se$ and $Li_{\delta}Cu_{2-x}Se$. Multiple samples and measurements are shown together, showing that the variation is significantly less than the difference achieved by changing the compositions.

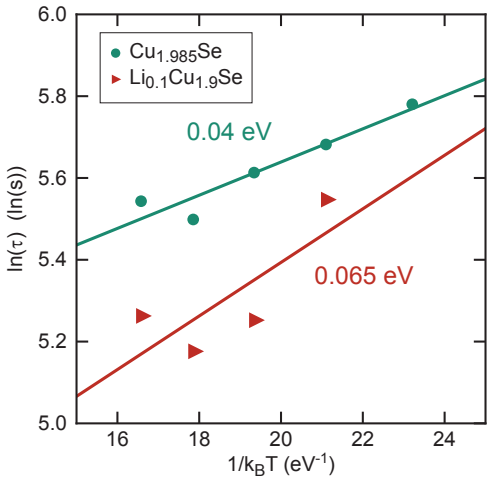

Figure S2: Comparison of the activation energy for ionic diffusion measured by fitting ionic relaxation times. The relaxation times were measured by a method described by Yokota [1] at the Shanghai Institute of Ceramics. A DC current is stressed on the sample to induce a polarized Cu ion profile. Two Pt wire leads were placed on the sample with a distance of ≈ 5 mm, which were used to record the potential variation induced by the DC current. The relaxation time represents the time to revert to 0 V after turning off the current. Measurements were done under static Ar atmosphere.

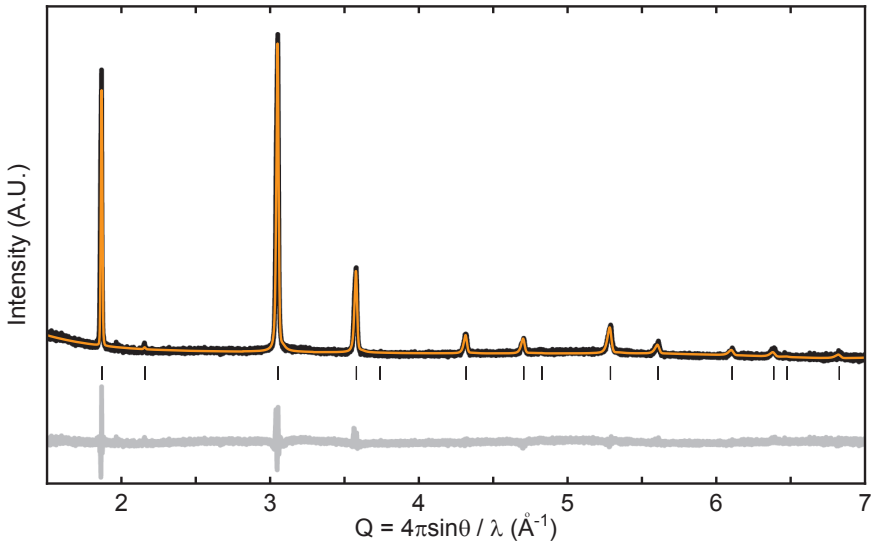

Figure S3: Rietveld refinement of $Li_{0.09}Cu_{1.9}Se$ at 490 K. The refined parameters are shown in Table S1. Only the main phase was taken into account for the refinement.

Table S1: Parameters for the refinement of $Li_{0.09}Cu_{1.9}Se$ at 490 K. Space group is $Fm\bar{3}m$.

	Cu (8*c*)		Cu (32*f*)			Se (4a)			
a (Å)	Occupancy	U_{iso} (Å^2)	x in (x,x,x)	Occupancy	U_{iso} (Å^2)	U_{iso} (Å^2)	R_p (%)	R_{wp} (%)	χ^2
5.8205	0.710	0.0613	0.3846	0.0605	0.084	0.0319	6.2	6.1	1.21

References

1. Yokota, I. On the Electrical Conductivity of Cuprous Sulfide: A Diffusion Theory. *Journal of the Physical Society of Japan* **8,** 595–602 (1953).